Variational Methods for Nuclear Systems with Dynamical Mesons

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Abstract

We derive a model Hamiltonian whose ground state expectation value of any two-body operator coincides with that obtained with the Jastrow correlated wave function of the many-body Fermi system. Using this Hamiltonian we show that the variational principle can be extended to treat systems with dynamical mesons, even if in this case the concept of wave function looses its meaning.

Variational methods, based on the Fermi Hyper Netted Chain (FHNC) expansion [1, 2, 3], also connected with the Correlated Basis Function perturbation theory[4, 5], have in the last years provided a satisfactory description of the static properties and of the response functions of the nuclear matter[6] and of other quantum fluids like, e.g., the liquid ^3He.

The FHNC approach is however seemingly constrained to non relativistic potential theories, where the wave function concept makes sense and correlated wave functions of the type:

$$\psi_G = \hat{G}\phi(r_1, \ldots, r_A), \tag{1}$$

with $\phi(r_1, \ldots, r_A)$ being a Slater determinant and $\hat{G}$ being a correlation operator, can be used. The simplest of such correlation operators is given by the Jastrow Ansatz

$$\hat{G}_J = \prod_{i<j}^{A} f(r_{ij}). \tag{2}$$

In this letter we show that a variational method exists that is able to properly account for systems where the wave function concept breaks down: this happens for instance when dealing with dynamical meson exchange, a process not reducible to the frame of a potential theory, which will be the main topics of the present letter. The same underlying idea however could be applied to other fields in solid state physics (Ising and Hubbard models, for instance), and could provide further improvements in the customary FHNC calculations since our approach, as we shall see, can allow an energy-dependence in the correlation function.

In this letter we wish to outline the general idea, namely the translation of the variational problem from the setting of a trial wave function to the setting of a trial Hamiltonian. Thus we are able to overcome the constraint represented by the need of defining a wave function, so allowing the treatment of dynamical meson exchanges (or similar situations). We exemplify this treatment for the case of the Jastrow correlated wave function.

We avoid here technical difficulties by confining ourselves to nonrelativistic nucleons coupled to mesons but disregarding for instance state-dependent correlations; more detailed problem will be dealt with separately in subsequent papers.

To achieve our goal, we have to solve three problems:

1. to embody the variational principle into a formalism able to handle effective Hamiltonian, [7, 8]

2. to translate the variational wave function (we will limit ourselvs to the Jastrow Ansatz) into a Hamiltonian formalism,

3. to find an effective Hamiltonian with nucleons only as true degrees of freedom but exactly including the dynamical meson exchange[9, 10, 11].

These items are nicely expressed in the Feynman Path Integral language [7]. Concerning item 1 the variational procedure is derived as follows. Let $H(\psi^\dagger, \psi)$ be the Hamiltonian of a many-body system and

$$
Z = \int \mathcal{D}[\psi^\dagger, \psi] e^{-\int_0^\beta d\tau\, H(\psi^\dagger, \psi)} , \tag{3}
$$

the partition function. The ground energy of the system is

$$
E_0 = - \lim_{\beta \to \infty} \frac{\log Z}{\beta} . \tag{4}
$$

The partition function is of course defined in the euclidean world, so that the Feynman-Kaç measure and consequently the integral in (3) are well defined.

We introduce a weighted average on the space of the Feynman-Kaç-integrable functions [12] as

$$
< f >_{H_0} = \frac{\int \mathcal{D}[\psi^\dagger, \psi] e^{-\int_0^\beta d\tau H_0} f(\psi^\dagger, \psi)}{\int \mathcal{D}[\psi^\dagger, \psi] e^{-\int_0^\beta d\tau H_0}} , \tag{5}
$$

where $e^{-\int_0^\beta d\tau H_0}$ plays the role of a weight function. Actually H_0 will be interpreted as a suitably chosen model Hamiltonian either solvable or at least easily manageable. It is worth stressing that H_0 is not necessarily the representation in the Bargmann-Fock space of a true Hamiltonian (i.e. an energy-independent hermitian operator bounded from below): it is only requested to be real and positive-definite in the euclidean world. Thus an explicit frequency dependence of H_0 can be allowed.

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Using (5) and the inequality $< e^{-A} > \geq e^{-<A>}$ we find

$$
\begin{aligned}
Z &= < e^{-\int_0^\beta (H - H_0)d\tau} >_{H_0} \int \mathcal{D}[\psi^\dagger, \psi] e^{-\int_0^\beta d\tau H_0} \\
&\geq e^{-<\int_0^\beta (H - H_0)d\tau>_{H_0}} \int \mathcal{D}[\psi^\dagger, \psi] e^{-\int_0^\beta d\tau H_0} ,
\end{aligned} \tag{6}
$$

from which the result

$$
E_0 \leq E_{var} = \lim_{\beta \to \infty} \frac{< \int_0^\beta d\tau H >_{H_0}}{\beta} , \tag{7}
$$

easily follows.

As for H_0, H is not requested to be hermitian or energy-independent: it only needs to be real in the euclidean world. Thus (7) applies to effective Hamiltonians as well, provided they are real after a Wick rotation.

This procedure can be applied to a meson theory provided an effective Hamiltonian is derived; on the other hand we are free to choose a suitable H_0. This makes the difference with the variational approach: there we guess the ground state wave function, here we guess an unperturbed Hamiltonian. How could we force the two approaches to coincide?

Now we are ready to better formulate question 2): we look for an operator H_0 such that the Jastrow wave function F will be its ground state. Presently we need something less, namely that E_{var} coincides with the expectation value of H on the Jastrow wave function ψ_J of eqs. (1,2)

Let us consider the following model Hamiltonian:

$$
H_0^{(J)} = \Delta \sum_{k < k_F} a_k^\dagger a_k + \frac{\Delta}{2} \sum_{kpq} \lambda(q) a_{k+q}^\dagger a_k^\dagger a_{p-q} a_p . \tag{8}
$$

We claim that

$$
E_{var}^{(J)} = \frac{< \psi_J | H | \psi_J >}{< \psi_J | \psi_J >} , \tag{9}
$$

provided the correct link between $\lambda(q)$ and $f(r_{12})$ is found.

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We will present here only the proof that the above equality holds for the expectation value of the potential energy, namely

$$V_{var}^{(J)} = \lim_{\beta \to \infty} \frac{< \int_0^\beta d\tau V >_{H_0}}{\beta} = \frac{< \psi_J | V | \psi_J >}{< \psi_J | \psi_J >} . \qquad (10)$$

Since this result will be true independently from the particular V present in the Hamiltonian, it implies that the diagonal part of the two-body density matrix either derived from our model Hamiltonian or from the Jastrow Ansatz will coincide. Consequently the one-body density matrix will do the same and the kinetic energies will also coincide.

We shall show that $V_{var}^{(J)}$ is given by the sum of the FHNC diagrams.

Let us expand the lhs of eq. (9) in Goldstone diagrams using the bilinear part of $H_0^{(J)}$ as unperturbed Hamiltonian. A simple analysis shows that at each order the quantity $V_{var}^{(J)}$ is independent from Δ (a nth order diagram has $n \ \Delta\lambda(q)$ terms and n energy denominators: since each of the latter $\propto \Delta$, then all Δ's cancel). On the contrary the Green's functions of the theory depends upon Δ and becomes singular when $\Delta \to 0$.

Let us now show the connection between the perturbative expansion of $V_{var}^{(J)}$ and the FHNC diagrammatical expansion of $< \psi_J | V | \psi_J > / < \psi_J | \psi_J >$.

We consider a Feynman diagram of the expansion of $< V >_{H_0}$ (a first-order diagram is shown in fig.1a). The solid lines (unperturbed Green's functions) are given by

$$\mathcal{G}_0(k, k_0) = \frac{\theta(k - k_F)}{k_0 + i\eta} + \frac{\theta(k_F - k)}{k_0 - \Delta - i\eta} \qquad (11)$$

We split $\mathcal{G}_0$ into two pieces:

$$\mathcal{G}_0(k, k_0) = g_0(k, k_0) + K(k, k_0) \qquad (12)$$

$$g_0(k, k_0) = \theta(k_F - k) \left\{ \frac{1}{k_0 - \Delta - i\eta} - \frac{1}{k_0 + i\eta} \right\} \qquad (13)$$

$$K(k, k_0) = \frac{1}{k_0 + i\eta} \qquad (14)$$

Next we sort new diagrams from the Feynman graph by expanding it by means of (12). In our example three graphs are generated (fig.1b): single

lines now represent g_0 lines and double lines K lines. Next we carry out the frequency integration, that will be in general elementary if λ is energy-independent, so coming to Goldstone diagrams. In each of them the K lines (which are momentum-independent) cannot leave any trace and are shrinked to points. Tadpoles also translate into constants and are also represented as points. The result is shown in fig. 1c.

All the FHNC diagrams can be reproduced in a similar way. In fact the frequency integration reduces the product of the energy denominators in a given diagram to a factor $m\Delta^k$ (with m integer, k being the order of the diagram), and this factor is canceled by the Δ^k coming from the interaction terms. Thus the K line can only influence the integer m. The g_0 lines after the frequency integration become θ-functions. We remind the reader that the Pauli correlation line of the FHNC diagrams corresponds to the Fourier transform of the θ-function, i.e.

$$l(k_F x) = \frac{\nu}{\rho} \int \frac{d^3 p}{(2\pi)^3} \theta(k_F - p) e^{i\mathbf{k}\cdot\mathbf{x}} . \tag{15}$$

The multiplicity factors ν coming from spin-isospin summations necessarily coincide both in the present approach and in the FHNC formalism, since they come from the counting of closed loops; the powers of the density, coming from integrations over single g_0 lines, also coincide with those of FHNC for dimensional reasons.

So far we have demonstrated the topological equivalence between the FHNC diagrams and those of the present theory. It remains clarify the relation between the correlation function $h = f^2 - 1$ of FHNC theory and the "potential" λ and then to verify that the coefficients carried by the diagrams coincide in the two expansions.

For these purposes we follow the derivation of FHNC diagrams given in [13]. There the two-body operator $U = 2\log f^2$ is introduced and a fictitious time dependence is assigned both to U and to the potential V with the results

$$< \Phi_0|V e^U|\Phi_0 > = < \Phi_0|T \int_0^1 V(t) e^{\int_0^1 U(t)dt}|\Phi_0 > . \tag{16}$$

Next, in ref.[13] the r.h.s. of the above equation has been expanded by means of the Wick theorem, and the FHNC diagrams originally derived in ref.[1] are recovered.

Now, within the present approach, let us consider the Feynman-Kaç integral

$$\int \mathcal{D}[a_k(\tau), a_k^\dagger(\tau)] e^{-\int_0^\beta H_0^{(J)}(\tau)d\tau} \int_0^\beta V(\xi)d\xi \ , \tag{17}$$

for our infinite system: since the "unperturbed part" of the model Hamiltonian has the Fermi gas Slater determinant $|\Phi_0>$ as a ground state as in (16), we can reinterpret (17) as

$$< \Phi_0|T \int_0^\beta V(\xi)d\xi e^{-\Delta \int_0^\beta \lambda(\tau)d\tau}|\Phi_0 > \ . \tag{18}$$

Since the physical quantities we are interested in are independent of Δ, we can put $\Delta = \frac{1}{\beta}$ and make the replacement $\tau \to \tau/\beta$ to recover (16) provided we identify U with $-\lambda$ in configuration space. Next we take the limit $\beta \to \infty$ (and consequently $\Delta \to 0$) in order to apply (4) , (6) and (7). Since the value of Δ is immaterial, the equivalence between the FHNC development and the perturbative expansion of our model Hamiltonian is proved. A similar proof can be done for the kinetic energy part of the Hamiltonian.

Finally, in [13], it is shown that the ladder series of fig. 2 can be summed explicitly at the prize of redefining U. The diagram structure being identical, we can do the same in our case by means of the identification

$$h = e^{-\lambda} - 1 \ , \tag{19}$$

which, we remind, is justified in the limit $\Delta \to 0$.

This completes the second step of our program. Finally, to apply the previous results to pion physicis, we need an effective Hamiltonian containing fermions only, but also accounting for pion exchanges. In the context of QFT an effective action has been derived in ref. [11]. Following the same path we can write a lagrangian density of the form

$$\mathcal{L} = \mathcal{L}_N + \mathcal{L}_\pi + i\psi^\dagger(x)\Gamma(x)\psi(x)\phi(x) \tag{20}$$

$\mathcal{L}_N$ and $\mathcal{L}_\pi$ being the free lagrangians for nucleon and pion fields respectively and Γ a spin-isospin operator (plus eventually derivatives) and then the corresponding generating functional (the partition function in the Minkowski world), here for simplicity with fermionic sources only:

$$Z[\eta, \eta^\dagger] = \int \mathcal{D}[\psi, \psi^\dagger, \phi] e^{i \int dx [\mathcal{L} + \psi^\dagger \eta + \eta^\dagger \psi]} \tag{21}$$

Since the pionic field is at most quadratic in the exponent, the integral over $\phi(x)$ is gaussian and can be carried out explicitly, getting

$$Z[\eta, \eta^\dagger] = \int \mathcal{D}[\psi, \psi^\dagger] e^{iS_{\text{eff}} + i \int dx (\psi^\dagger \eta + \eta^\dagger \psi)} \ , \tag{22}$$

where

$$S_{\text{eff}} = \int dx \, dy \psi^\dagger(x) G_0^{-1}(x-y) \psi(y) \tag{23}$$

$$-\frac{1}{2} \int dx \, dy \psi^\dagger(x) \Gamma(x) \psi(x) D_0(x-y) \psi^\dagger(y) \Gamma(y) \psi(y),$$

G_0 being the free fermion propagator and D_0 the (fully dynamic) pion propagator

$$D_0(x-y) = \int \frac{d^4q}{(2\pi)^4} e^{iq\cdot(x-y)} \frac{1}{q_0^2 - \mathbf{q}^2 - m_\pi^2} \ , \tag{24}$$

The last step is to apply eq. (6) and (7) to the action (23). Thus first we go to the euclidean world, so that D_0 becomes real and bounded from below. Next we can use (7), since the q_0 dependence in D_0 does not prevent eq. (7) from holding, and we expand diagrammatically the average value of the (euclidean) action S_{eff} using $H_0^{(J)}$ as model Hamiltonian.

The diagrams so obtained have the same topological structure as the standard FHNC diagrams previously discussed, provided the time variable is added for the external points. Thus these diagrams can also be summed up by means of the usual FHNC technology, but now the constant Δ is no longer irrelevant: in fact in one energy denominator (namely the one of the meson) it is compared with a finite quantity (the meson mass). Thus Δ can be regarded as an extra variational parameter.

A more realistic *variational* Hamiltonian than $H_0^{(J)}$ should be used in connection with effective Hamiltonians of the type discussed above. The interaction term in $H_0^{(J)}$ should be modified to include state–dependent correlation effects present in a realistic $\hat{G}$[3]. Moreover, a time (or frequency) dependence could be introduced in λ, which would imply adding a time dependence in the internal points of the FHNC diagrams, or in other words to consider time dependent correlations. Work in this direction is in progress.

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Figure Caption

1. 1a A first order (with respect to λ) Feynman diagram.

   1b The diagrams obtained from 1a by means of eq. (12).

   1c The corresponding FHNC diagrams.

2. The ladder series corresponding to eq. (19)